ELECTRON PHYSICS

LAB GUIDE

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Introduction

The Electron Physics Group has ongoing research efforts in electron collision physics including electron-surface interactions, electrons microscopy, surface magnetism, electron interaction theory, electron polarization phenomena, electron-atom collisions, and electron optics and instrumentation. The wide applicability of electron-based measurement technologies allows us to contribute to the solution of many diverse scientific and technological problems.

This year we have continued to increase and focus our efforts toward the study of microscopic phenomena and their influence on the macroscopic properties of surfaces. As in the recent past, a major emphasis is on magnetic phenomena and structure. We are in the process of adding a scanning Auger microprobe facility to our effort which will greatly increase our capabilities in the study of magnetic microstructure. Additionally, most of our experiments are being adapted to the use of the technique of molecular beam epitaxy to grow thin over-layer films, permitting us to study interfacial phenomena.

The Electron Physics Group is a highly interactive group with many collaborative efforts both inside and outside of NIST. The external collaborations include joint efforts with researchers at universities, national labs, and industrial labs, as well as international collaborations.

We value very highly our postdoctoral fellows and visiting scientists and encourage prospective candidates to apply.

This booklet is to help you to get to know us, and what we do, better. If you would like more information on any topic, we would be happy to provide it.

Robert J. Celotta
Group Leader
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Electron-Atom Collision Studies Using Optically State-selected Beams

J.J. McClelland, M.H. Kelley and R.J. Celotta

The general aim of this project is to apply the technology of the GaAs polarized electron source developed in the Electron Physics group to the study of crossed-beam atomic collision physics. In particular, our interests lie in the investigation of low energy electron scattering from alkalis, such as sodium. These atoms are particularly interesting because they have a single outer electron which can be spin-polarized, via optical pumping, either parallel or anti-parallel to the incident electron polarization. By measuring parallel and anti-parallel scattering cross sections, one can resolve the scattering process into two independent channels—the singlet and the triplet. These two channels behave very differently in the presence of the exchange in low energy collisions.

1 Near Threshold Ionization

Our first set of measurements were done on the spin dependence of near-threshold electron impact ionization[1]. In this experiment, sodium atoms were optically pumped prior to the collision so that a beam of ground state atoms with 5/8 polarization was produced. The energy dependence of the ionization of these atoms was measured for incident electron spin parallel and anti-parallel to the atomic polarization. The resulting spin asymmetry was compared with theoretical predictions of either the Coulomb-dipole or the Wannier model for threshold ionization. Comparison is particularly easy in this case because the Coulomb dipole model predicts oscillations in the spin asymmetry while the Wannier model predicts no dependence on energy. Our measurements showed that there are no oscillations outside the experimental uncertainty and hence the Wannier model is fully sufficient to explain the experimental results.

2 Optical Pumping

In the process of developing the methods for optical pumping used in the ionization experiments, we found that is was very important to understand several aspects of the optical pumping process in detail. The basic mechanism was understood: circularly polarized laser light is tuned to the $F = 2 \rightarrow F = 3$ hyperfine transition of the $3S_{1/2} \rightarrow 3P_{3/2}$ sodium D_2 line, causing $\Delta M_F = +1$ transitions and resulting in a pileup of population in the $M_F = +2$ ground state and $M_F = +3$ excited state. But several groups had reported anomalously large losses to the $F = 1$ ground state, which is not pumped by the laser. Such losses can destroy the ground state atomic polarization by reducing the number of atoms which make it to the $M_F = +2$ state. Thus we felt it was necessary to probe this loss process. This we did both theoretically, solving numerically a multilevel version of the optical Bloch equations,

and experimentally using a two-laser, two-lock-in-pump-probe arrangement[2]. The measured and calculated fractional increase in the $F = 1$ population resulting from this study allowed us to put a firm value of 0.609 ± 0.018 on the net polarization of our atomic ground state.

3 Spin-polarized Superelastic Scattering

Some of the experiments currently under way involve investigating the role played by spin in the inelastic scattering of electrons from sodium. This we do by studying the inverse process, namely superelastic scattering, from the first excited state Na($3P_{3/2}$). In this type of experiment, we move the laser to intersect the atom beam at the scattering center, and observe only those electrons which gain the energy of the excited state (2.1 eV) in the scattering process. Since superelastic scattering is rigorously related to inelastic scattering as the time-inverse process, we can probe the inelastic spin-dependent cross section with a high degree of state selectivity and also with a good signal-to-noise ratio, since there are very few background electrons at energies higher than the primary beam energy.

Superelastic measurements have been conducted with both linearly polarized and circularly polarized optical pumping. The linearly polarized work[3] provided an interesting example of the "fine structure" effect, in which a spin asymmetry is observed in scattering spin polarized electrons from atoms with no net spin-polarization. Though this has the appearance of being due to the spin-orbit effect, it is really driven solely by the exchange interaction and the fact that the fine structure of the Na $3P$ state is resolved.

With circularly polarized excitation, the optical pumping creates spin-polarized pure angular momentum states of the target atom for the spin-polarized electrons to scatter from. This allows us to resolve the scattering process not only into triplet and singlet channels, but also into different angular momentum channels. The angular momentum partitioning is characterized by the quantity $L_\perp$, i.e. the angular momentum transferred in the collision perpendicular to the scattering plane. $L_\perp$ has different values for the singlet and triplet channels, and our spin-polarized electron beam allows us to measure these independently. Recently, we have completed a set of measurements of singlet and triplet $L_\perp$, as well as the triplet to singlet ratio, over the angular range 10° - 120° at energies of $2eV$, $17.9eV$ and $52.3eV$.[4,5,6] Comparison with well established calculations has shown some interesting differences, which will hopefully lead to new insights in the field.

4 Theory of Spin-polarized Superelastic Scattering

In order to make full use of our data, we have also done work on a theoretical framework for analyzing superelastic collisions with polarized electrons.[7] Using the density matrix formalism, we have cast the problem in the same general form used successfully to analyze alignment and orientation in unpolarized collisions. The three parameters

$L_\perp$, P_{lin} and γ are generalized to reflect singlet and triplet contributions, and a general expression for the scattering intensity is derived for an arbitrarily prepared atom and an electron with any polarization. This work will hopefully prove useful in analyzing a quite general class of experiments.

5 Elastic Scattering

Elastic scattering experiments are also under way as part of our state-selected scattering program. As in the case of the ionization work, the atoms are optically pumped before the interaction region to make spin-polarized ground states. Spin "up" or spin "down" electrons scatter from these atoms, and the scattered electrons are detected as a function of the four possible orientations of the electron and target. By keeping track of the four channels—"parallel up", "parallel down", "anti-parallel up" and "anti-parallel down"—we have been able to simultaneously observe exchange and spin-orbit effects for the first time.[8] This should provide new insights into the difficult theoretical problem of calculating electron scattering when neither the exchange nor the spin-orbit interaction can be ignored.

Our current efforts consist of work towards a theoretical understanding of the above mentioned elastic data, and also measurements using other incident electron energies and at other scattering angles. Plans for the future involve measurements of other atomic targets, addition of energy analysis so we can investigate other transition in sodium and also inclusion of spin analysis in the detection of the scattered electrons. Achieving this will allow a truly "complete" measurement of all quantum phases and amplitudes which determine the scattering.

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Angle and Spin Resolved Inverse Photoemission Studies of Unoccupied Valence Electronic Structure

M.W. Hart, D.T. Pierce and R.J. Celotta

In recent years we have applied the spin polarized electron source developed in this group to the study of ferromagnetic metal surfaces. By coupling this low energy spin polarized source with a UHV chamber equipped with a sample manipulator, an Auger spectrometer, and a LEED system a variety of unique experimental techniques have been employed to investigate the magnetic, chemical, and electronic properties of metal surfaces.[1,2] Currently, we are focusing on a spin polarized inverse photoemission (SPIPES) technique to study some transition metal surfaces.[3]

Inverse photoemission compliments photoemission studies by yielding energy and momentum resolved information about the unoccupied band structure at the surface. An electron incident upon the sample can undergo a radiative transition and become bound in a vacant orbital of the solid. The flux of 9.7 eV photons emitted from the sample is measured as a function of the energy, angle of incidence, and spin of the electrons. Since the energy, momentum, and spin are conserved, the final state is well defined. Because of its spin selectivity, SPIPES is applicable to a large number of areas of current interest in ferromagnetic materials.

We have recently completed an SPIPES investigation [4] of the clean Ni(001) surface and the c(2x2) absorption systems O/Ni(001) and S/Ni(001). For clean Ni(001), we found a minority-spin character for the unoccupied 3d band, but an essentially non-magnetic character for the Ni 4sp band. These spin-dependent results confirm previous spectral assignments made for Ni(001).[5] No spin dependence of the Ni(001) image potential surface state was found.

Our investigations of Ni(001) chemisorption yielded surprising results. No evidence was found for a c(2x2) oxygen-induced antibonding state at the surface Brillouin zone center, Γ, which is in direct contradiction with recent experimental[6], and theoretical[7] results. The chemisorbed oxygen does not significantly alter the intrinsic magnetization of the observed minority-spin 3d spectral peak. The chemisorbed sulfur overlayer produces a small intensity enhancement at the Ni 3d inverse photoemission peak, and reduces the observed spin dependence of the peak by four-fold. These variations suggest the possible existence of a sulfur-induced unoccupied state of majority spin character just above the Fermi level at Γ. Such a state would play a central role in the mechanism by which sulfur destroys surface magnetism.

We are currently investigating the electronic and magnetic properties of ultra thin epitaxial metallic films deposited on metallic substrates. By observing the spin resolved unoccupied band structure we hope to test recent theoretical predictions [8] as well as address fundamental questions concerning the magnetic character of some of these systems.[9]

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Scanning Tunneling Microscopy of Surfaces: Atomic Structure and Microstructure

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A scanning tunneling microscope (STM) is an instrument that produces high-resolution surface topographic maps of conducting or semiconducting materials. A STM has been shown[1] to have atomic lateral resolution and sub-atomic vertical resolution. The procedure for mapping surface structure[2] involves moving a conducting tip within a few angstroms of a voltage-biased surface to attain a measurable electron tunneling current (typically 1 nA) without touching the surface. The tunneling current is servoed to remain constant by providing an error correction to the tip-to-sample distance. The tip is scanned in a raster pattern across the surface of the sample providing topographic maps. The information gathered is actually a convolution of the electronic structure of the tip and of the scanned sample. However, because of the exponential decay of the tunneling probability with distance, only the last few atoms on the end of the tip interact with the sample (if it is extremely flat) and the tip can be considered to be an ideal probe. Furthermore, by varying the bias voltage, the electronic surface structure can be separated from and measured simultaneously with the physical topographic structure.[3]

The STM that we have constructed is housed in an ultra-high vacuum chamber that includes a sample introduction chamber and a sample characterization area (with the capabilities of Auger spectroscopy, LEED, ion sputtering, metal evaporation, and electron bombardment heating). The STM is mounted on a quartz plate (for thermal stability) that rests in a double-spring suspension sytem (for vibration isolation). The STM is composed of a xyz piezoelectric tripod for fine tip positioning in three dimensions and a piezoelectric/electrostatic clamping device for coarse sample positioning in two dimensions. The system is quite versatile (allowing for fast change of either tip or sample) and provides an excellent basis for experimental procedures.

In the process of building the scanning tunneling microscope, we initially operated the instrument with a glass bell jar cover before adding the bakeable stainless steel bell jar necessary for surface science experiments. During this time we examined the topographies of two optical surfaces—a ruled, grating replica and a diamond-turned gold mirror.[4] The scanned areas of the grating replica ($2.2\ \mu m \times 2.4\ \mu m$—quite large for a STM) reproduced the periodic grating structure ($0.46\ \mu m$ ruling) with amplitudes of $20-30\ nm$. The structure on the diamond-turned mirror (measured to rather high resolution: ~ 10 Å lateral, ~ 1 Å vertical) exhibited a periodic component that corresponded to the spacing of the tool cuts ($\sim 100\ nm$) as well as non-periodic structure that is related to other aspects of the machining process, such as metal build-up on the cutting tool.

The STM is now fully operational in the ultra-high vacuum chamber and atomic resolution has been obtained. The atomic pattern of the 7×7 reconstruction on Si(111) has been observed over a fairly large area ($30 \times 30\ nm$) which included ~ 100 unit cells. The resolution attained with the microscope was $\sim 0.5\ nm$ lateral and $\sim 0.01\ nm$ vertical.

Our primary experimental interest is the characterization of thin film growth structures. The microscope will be used to examine changes in the surface structure of various materials after deposition of submonolayer and multilayer films of different evaporants. We will measure changes in atomic structure such as surface reconstructions and larger scale surface changes such as the formation of island structures. We will attempt to perform the evaporation *in situ* in order to scan the same area of the surface before and after evaporation and thereby correlate changes in the surface after deposition to the character of the surface before deposition (e.g. reconstructions, defects, steps, etc.).

Another interest involves working jointly with the SEMPA project (discussed in this manual) to provide characterization of magnetic systems that are of scientific interest. In order to understand the behavior of two-dimensional magnetism in thin films and surfaces, for example, as determined with the SEMPA technique, it is essential to characterize the surface with as high a resolution as possible. This will be accomplished with the STM by simultaneously measuring the physical structure with the electronic structure in order to determine the 'flatness' and the composition of the thin films. We will also pursue the possibility of adapting the STM to be sensitive to the spin of the tunneling electron, thereby having the capability to image magnetic surface structure with high resolution. There are numerous interesting systems that could be examined with such an instrument, including the growth and characterization of one- and two-dimensional ferromagnetic structures.

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Electron Transport Theory

D.R. Penn

(a) The techniques of spin polarized electron scattering and spin polarized electron detection have been utilized to produce valuable information relevant to magnetism in metals and related metallic glasses. Recently an experiment using both a polarized electron beam and spin polarized detection was reported.[1] Hence for the first time it is possible to carry out a detailed theoretical analysis of the spin dependent scattering process. Our analysis concludes that free electron-like Stoner excitations (FESE) contribute significantly to the scattering process. A FESE is an electron-hole pair excitation consisting of a d hole of given spin and an electron in a free electron-like state of opposite spin. The usual type of Stoner excitation in which the electron is in a d state will be referred to as a d electron Stoner excitation (DESE).

Within the model used to analyze the data two rather surprising conclusions can be drawn: (1) Exchange scattering events are as important as non-exchange scattering, and (2) Electron-hole pair excitations that have free electron like final electron states are somewhat more likely than those with d electron final states. Thus, creation of a FESE is more likely that a DESE, the usual type of Stoner excitation.

(b) A new general formula has been proposed[2] for determining electron inelastic mean free paths (IMFPs) for 200–2000 eV electrons in solids. The new formula is based on separate IMFP calculations for 27 elements and 4 compounds using an algorithm we recently developed.[3] This formula is believed useful for determing the IMFP dependence on electron energy for a given material and the material-dependence for a given energy. The new formula should also be a reasonable guide to electron attenuation lengths which have been difficult to determine with the needed accuracy.

(c) Metastable He atoms incident on Ni metal produce Auger electrons from the Ni. The number produced depends on the relative spin of the He atoms and the Ni. The normalized difference increases as the kinetic energy of the Auger electrons increases.[4] We have developed a theory of the asymmetry. In contrast to the usual interputation we have found the s-p electrons to be of crucial importance. Whereas the d electrons carry the main magnetic moment the s-p electrons have the largest overlap with the He atoms. Our theory[5] shows that the asymmetry is a direct measure of the exchange scattering amplitude in a process involving both s-p and d electrons. Good agreement with experience[4] is obtained.

The interaction between two test charges in a solid can be described in terms of a total dielectric function that includes electronic and lattice polarization. Stability requirements place restrictions on the dielectric function. We have generalized these restrictions, which have previously been determined for the case of a uniform media, to the inhomogeneous case and discussed some implications for superconductivity. We have derived a total dielectric function for the electron-lattice system in the mean field approximation and explicitly constructed its inverse. The low-lying poles of e^{-1} give the correct phonon frequencies as determined by the usual dynamical matrix.

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Scanning Electron Microscopy with Polarization Analysis (SEMPA)

J. Unguris, M.R. Scheinfein, R.J. Celotta and D.T. Pierce

Scanning Electron Microscopy with Polarization Analysis (SEMPA) is a new technique that we have developed and are using to look at very small, submicron magnetic structures.[1,2,3,4]

When an electron beam is incident upon a ferromagnetic material spin polarized secondary electrons are generated.[5,6] The electron spin polarization of the secondary electrons is simply proportional to the spin polarization of the valence electrons in the solid. Therefore a measurement of the polarization of the secondary electrons yields a direct measurement of the magnetization in the region of the sample probed by the incident electron beam. In order to measure magnetic structures with high spatial resolution we have added electron spin polarization analyzers to a scanning electron microscope. We can therefore not only obtain the usual topographic map of a material, but in addition we simultaneously and independently image the magnetic microsctructure. The spatial resolution of the two images is the same and approximately equal to 10 nm.

SEMPA has several unique capabilities that set it apart from other magnetic imaging techniques: First, SEMPA offers the highest spatial resolution for observing magnetic microstructures in reflection. (Only Lorentz imaging using a TEM and thinned specimens has better resolution). Second, SEMPA measurements of magnetic microstructure are independent of topography, but the magnetic and topographic maps are measured simultaneously. This feature helps in understanding the relationships between topographic and magnetic structures. Third, SEMPA is a direct measurement of the magnetization vector. We therefore image both the magnitude and direction of magnetization. And finally, because the escape depth of the secondary electrons is about 5 nm, SEMPA is a relatively surface sensitive technique. This makes it very useful for the study of magnetism at surfaces and in thin films.

Because SEMPA is still a relatively new technique, most of the current work has involved both developing and perfecting the SEMPA instrumentation and performing a series of exploratory experiments to test the capabilities of SEMPA. Perhaps the biggest breakthrough in instrumentation involved the development of a new kind of electron spin polarization analyzer.[7] This detector, which is based on the spin orbit interaction in the scattering of 150 eV electrons from an evaporated Au film, is much more compact and simpler to use than previous detectors. Addition of the polarization analyzers to the electron microscope was therefore fairly straightforward and, more importantly, did not degrade the microscope performance.

So far we have successfully imaged magnetic microstructures in the following materials: (i) Fe -3 % Si single cyrstals, (ii) Permalloy thin films, (iii) Permalloy thin film recording heads (provided by Control Data Corp.), (iv) CoNi sputtered films (provided by Kodak), (v) various Fe-based metglasses (provided by NSWC and Allied Chemical), and (vi) evaporated Fe films that were only a few monolayers thick (this work was in collaboration with Naval Research Lab).

We are planning to use SEMPA to investigate a variety of micromagnetic systems in greater detail. These systems will range from ones that have immediate technological applications, such as, magnetic recording media, thin film memory devices,

magnetic domain dynamics, new fine grained magnets for electrical motors, or the magnetism of layered materials, to systems that are of scientific interest such as two-dimensional magnetism in thin films and surfaces, magnetic structure within domain walls, or the domain structure of submicron particles.

We are also in the process of adapting another electron microscope for spin polarization analysis. This microscope will be a scanning Auger microprobe and will therefore be able to give us a map of the chemical composition of the surface along with the topographic and magnetic images.

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Polarized Photoemission Studies of Magnetic Systems

D.P. Pierce and R.J. Celotta

We have been working in collaboration with AT&T Bell Laboratories and Brookhaven National Laboratory to employ spin-polarized, angle-resolved photoemission to study surface magnetism. This pilot effort has been greatly expanded in scope by the addition of a large number of prominent collaborators to form a Materials Research Groups (MRG). The NSF-supported MRG consists of eleven principal investigators from the following institutions: AT&T Bell Labs, NSLS-Brookhaven National Laboratory, Argonne National Laboratory, Northwestern U., Rice U., U. of Texas at Austin, Naval Research Laboratory, and U. of California at Irvine, and our own Group at NIST. The focus of the effort will be to study both bulk materials and epitaxial ferromagnetic mono-, bi-, tri- and multi-layer materials. Investigations will include ground state magnetic properties, testing local density theory predictions, surface magnetic critical phenomena, spin-dependent photo-excitation, and energy-and-wave-vector-resolved electron spectroscopy. Because of the increasing importance of interfaces and multi-layered structures, the experimental station will include a molecular beam epitaxy appartus for fabricating unique magnetic multi-layered structures. A component of this research will be aimed at improving the photon flux available from the U-5 beam port on the NSLS UV storage ring. Our MRG has been designated as an insertion device team and will be installing a new undulator to provide a greatly enhanced photon flux for use in spin-polarized photoemission experiments.

This effort in understanding exotic magnetic structures will complement our effort in magnetic microstructure (SEMPA) and physical and electronic microstructure (STM) and greatly enhance our ability to understand the macroscopic physical properties of matter through study of their microscopic structure.

Electron Optics

M.H. Kelley and M.R. Scheinfein

A feature common to many of the experimental programs in this group is the reliance on in-house development of electron optical instrumentation. There are two major directions taken in our work on electron optics. The first is the design and construction of electron optical systems whose operational characteristics satisfy the needs of specific applications. This includes the design of beam forming and transport optics, energy monochromators and analyzers, and imaging optics for electron microscopy. The second major task is to model realistically the operation of existing devices, including the effects of imperfections such as stray electric or magnetic fields, mechanical misalignments, space charge, etc.

We approach the design phase at several different levels of complexity. A preliminary design is found by combining electron lenses of standard geometries and optimizing the lens positions, diameters, and applied voltages to achieve the desired operating characteristics. At this stage, the operating characteristics are modeled using matrix transport techniques and the effects of aberations and space charge are typically neglected. Tabulated matrix elements are available for a wide variety of standard lenses. We use for our calculations those of Harting and Read[1] as well as matrix elements determined at NIST.[2] Once a preliminary configuration has been established which satisfies the specified operating criteria, the effects of aberations, space charge, etc., are investigated and the design modified, if necessary, to maintain the desired characteristics. If it is deemed appropriate, the accurate behavior of the system is then modeled numerically by solving the equations of motion for the electrons in the electric and magnetic fields of the device.

It is often desirable to attempt to model realistically the behavior of actual instruments including the effects of physical imperfections or stray external fields. We do this modeling numerically using the computing resources available to us at NIST. Essentially any system with cylindrical or plane symmetry can be reasonably well handled. Electrostatic potentials produced by the boundary conditions of the actual lens system are determined by solution of Laplace's equation, using either the method of successive over relaxation,[3] or the change density method.[1] Essentially any system with cylindrical or planar symmetry can be reasonably well handled. Magnetic fields arising from magnetic elements are determined using finile element methods.[4] Electron trajectories are then determined by integrating (three-dimensionally) the equations of motion (including relativistic corrections where appropriate) with a high order predictor corrector method.[3] Trajectories thus generated are used to predict the common properties of electron lenses with accuracies as good as 0.1% depending on the details of specific situations.

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PLEED Lab	B211/220	73723
Vacuum Assembly Room	B207/220	3723
JEOL Lab	A017/220	3759
STM Lab	A017/220	3759
Sample Prep Room	B215/220	73705
Field Emission Microscope Lab	A021/220	73474